

1-Nitropropane
108-03-2 | DTXSID1020980

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 129 °C

Global applicability domain: Inside

Local applicability domain index: 7.40e-01

Confidence level: 8.44e-01

Nearest Neighbors from the Training Set

Image not found

1-Nitropropane

Measured: 131

Predicted: 129

Image not found

2-Nitropropane

Measured: 120

Predicted: 124

Image not found

1-Propene, 3-nitro-

Measured: 128

Predicted: 125

Image not found

Propane, 2-methyl-1-nitro-

Measured: 141

Predicted: 140